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Numerical investigation of a fractional diffusion model on circular comb-inward structure

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Abstract

In this paper, the diffusion dynamics of particles on a circular comb-inward structure with different radial and tangential mobilities are studied. The Scott-Blair time-fractional memory model is exploited to incorporate the trapping process in the diffusion. A new formulation of particle flux is proposed which the numerical discretization is straightforward. The numerical scheme is based on the second-order $L2-1_\sigma$ formula for time stepping and uses the finite difference method for spatial approximations. The influences of involved parameters on the distribution of particles and the mean-square displacement (MSD) are investigated in detail. According to the model prediction, the diffusion of particles on the ring decreases with the smaller values of the fractional order α. Results also indicate that the radial and tangential mobilities exhibit the opposite effects on the MSD of particles.

Keywords: Anomalous diffusion, Circular comb structure, Memory kernels, Scott-Blair model

1. Introduction

Transport of particles on a comb-like structure often exhibits anomalous diffusion, namely the Fick's second law fails to model this particular diffusion due to the fingers [1–3]. The motion feature in such structure is that the diffusion occurs only on the backbone and inside the fingers, which needs to more efforts to mathematical formulation. Luckily, it was done nearly thirty years ago by modifying the diffusion coefficients with a Dirac-delta function [4]. In this work, a new idea by reformulating the flux for diffusion on a comb-like structure is proposed, which is motivated by the immersed boundary method [5] and convenient for numerical implementation.

The interest in studying diffusion on a comb-like structure is relevant for the problems of transportation and proliferation of cancer cells [6], the calcium transport inside spiny dendrites [7], and potential applications in surface charge convection on fluid drops [8] and so on. More recent years, there have been some attempts to model the anomalous trapping phenomena associated with the comb geometry, which may lead to the non-locality in time. Méndez and Iomin [9] proposed a generalization of the particle flux with the time fractional Riemann-Liouville derivative to describe transport in spiny dendrites. Sandev et al. [10] studied the Lévy processes on a fractal comb and a variety of memory kernels are discussed. Liu et al. [11] developed a fractional Cattaneo-type diffusive flux in comb structure. Subsequently, Fan et al. [12] extended the diffusion to a circular comb-like structure with anisotropic relaxation using the classical Maxwell-Cattaneo model. During the same period, this constitutive model was also used to consider the finite-velocity diffusion on a comb [13]. From the previous works, a special memory kernel, i.e. the Scott-Blair fractional memory kernel, is considered to study the anomalous diffusion on circular comb-inward structure with different mobilities.

The comb-inward model with round structure consists of a circular backbone and radial branches as shown in Fig. 1. The diffusion occurs in the tangential direction only at $r = r_0$. The diffusive flux

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$\overrightarrow{J} = (J_r, J_\theta)$ in radial and tangential directions in the polar coordinate is defined as follows

$$J_r = -D_r \frac{\partial P}{\partial r}, \quad J_\theta = -D_\theta \int \frac{1}{r}\frac{\partial P}{\partial \theta}\delta(r-r_0)dr, \tag{1}$$

where $P(r, \theta, t)$ is the two-dimensional distribution function, $\delta(r - r_0)$ is the shifted Dirac-delta function, D_r and D_θ are the diffusion coefficients, respectively. It is worth mentioning that this formulation of J_θ is inspired by the immersed boundary method [5] and one immediately obtains the classical flux on the boundary.

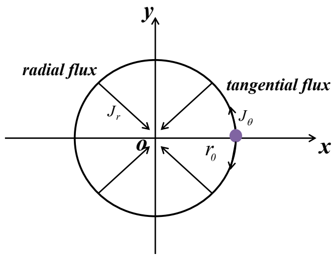

Fig. 1: Schematic drawing of the circular comb-inward structure.

Furthermore, in order to incorporate the memory effects for the transport dynamics of particles on the comb structure, which often means a convolution integral of the diffusive flux with a specific memory kernel [9, 14], we first consider the Scott-Blair fractional memory model given by [15]

$$J_r = -D_r \cdot {}_{RL}D_t^{1-\alpha}\Big[\frac{\partial P}{\partial r}\Big], \quad J_\theta = -D_\theta \cdot {}_{RL}D_t^{1-\alpha}\Big[\int \frac{1}{r}\frac{\partial P}{\partial \theta}\delta(r-r_0)dr\Big], \tag{2}$$

where ${}_{RL}D_t^{1-\alpha}$ denotes the time-fractional derivative in the Riemann-Liouville sense [16] defined as

$${}_{RL}D_t^{1-\alpha}P\big(r,\theta,t\big) = \frac{1}{\Gamma(\alpha)}\frac{\partial}{\partial t}\int_0^t \frac{1}{(t-\tau)^{1-\alpha}}P(r,\theta,\tau)d\tau, \quad 0<\alpha<1, \tag{3}$$

where $\Gamma(\alpha)$ is a gamma function.

2. Mathematical formulation

The continuity equation and the divergence operator can be written as

$$\frac{\partial P}{\partial t} + \nabla \cdot \overrightarrow{J} = 0, \quad \nabla\cdot = \Big(\frac{1}{r}\frac{\partial}{\partial r}r, \frac{1}{r}\frac{\partial}{\partial \theta}\Big). \tag{4}$$

Substituting the constitutive relation (2) into (4) yields the time fractional diffusion equation

$$\frac{\partial^\alpha P}{\partial t^\alpha} - D_r\frac{1}{r}\frac{\partial}{\partial r}\Big(r\frac{\partial P}{\partial r}\Big) - D_\theta\frac{1}{r}\frac{\partial}{\partial \theta}\Big(\int \frac{1}{r}\frac{\partial P}{\partial \theta}\delta(r-r_0)dr\Big) = 0, \tag{5}$$

where the time fractional derivative is the Caputo type definition, the units of D_r and D_θ are m^2/s^α. By introducing the dimensionless quantities: $t^* = t/T$, $r^* = r/r_0$. the nondimensional form of (5) is (the superscript $*$ is omitted for brevity)

$$\frac{\partial^\alpha P}{\partial t^\alpha} - d_r\frac{1}{r}\frac{\partial P}{\partial r} - d_r\frac{\partial^2 P}{\partial r^2} - d_\theta\frac{1}{r}\frac{\partial}{\partial \theta}\Big(\int \frac{1}{r}\frac{\partial P}{\partial \theta}\delta(r-1)dr\Big) = 0, \tag{6}$$

where the dimensionless numbers d_r and d_θ are defined as $d_r = D_rT^\alpha/r_0^2$ and $d_\theta = D_\theta T^\alpha/r_0^2$. The (6) is completed with the following initial and zero Neumann boundary conditions as

$$P|_{t=0} = \delta(r-1)\delta(\theta), \quad \frac{\partial P}{\partial \theta}\Big|_{\theta=-\pi} = \frac{\partial P}{\partial \theta}\Big|_{\theta=\pi} = 0, \quad \frac{\partial P}{\partial r}\Big|_{r=0} = \frac{\partial P}{\partial r}\Big|_{r=1+\epsilon} = 0, \tag{7}$$

where ϵ is a tiny outward extension for accommodate the source of particles at the boundary $r = 1$.

3. The numerical approach

The temporal discretization of the Caputo derivative employs the second-order $L2-1_\sigma$ formula proposed in [17]. The finite difference method is used for spatial discretization and the variable P is stored in the cell centers to deal with the reflecting boundary conditions [18]. Define $\tau = T/N_t$ and $t_n = n\tau$, $n = 0, 1, ..., N_t$, where τ refers to the time step size, the spatial domain is subdivided into rectangular cells of equal size in each direction $h_r = 1/N_r$, $h_\theta = 2\pi/N_\theta$, where N_r and N_θ are two positive integers. The fully-implicit second-order scheme for updating $\{P^{n+1}\}_{n=1}^{N_t-1}$ is given as

$$\{\mathcal{D}_t^\alpha P^{n+\sigma} - d_r \frac{1}{r}\nabla_r P^{n+\sigma} - d_r \Delta_r P^{n+\sigma} - d_\theta h_r L_r(r-1)\frac{1}{r^2}\Delta_\theta P^{n+\sigma} = 0\}\big|_{(i,j)}, \tag{8}$$

where $\sigma = 1 - \alpha/2$, the spatial difference operators are defined as

$$\nabla_r P = \frac{P_{i+1,j} - P_{i-1,j}}{2h_r}, \Delta_r P = \frac{P_{i+1,j} - 2P_{i,j} + P_{i-1,j}}{h_r^2}, \Delta_\theta P = \frac{P_{i,j+1} - 2P_{i,j} + P_{i,j-1}}{h_\theta^2}. \tag{9}$$

The function $L_r(\cdot)$ is the numerical approximation of the Dirac-delta function defined as [5]

$$L_r(l) = \begin{cases} \frac{1}{4h_r}\left(1 + \cos(\frac{\pi r}{2h_r})\right), & |l| < 2h_r, \\ 0, \quad |l| \geq 2h_r. \end{cases} \tag{10}$$

The variable $P^{n+\sigma}$ is defined as $P^{n+\sigma} = \sigma P^{n+1} + (1-\sigma)P^n$, which is second-order in time. The discrete Caputo derivative is given by

$$\begin{aligned} \mathcal{D}_t^\alpha P^{n+\sigma} &= \sum_{k=1}^{N_{\exp}} \widehat{w}_k V_k^n + \lambda a_0 (P^{n+1} - P^n), \\ V_k^n &= e^{-s_k\tau} V_k^{n-1} + A_k(P^n - P^{n-1}) + B_k(P^{n+1} - P^n), \end{aligned} \tag{11}$$

where $N_{\exp}$ is a positive integer, the other parameters in (11) are evaluated as

$$\begin{aligned} &\lambda = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)}, \quad a_0 = \sigma^{1-\alpha}, \quad \widehat{w}_k = \frac{1}{\Gamma(1-\alpha)} w_k, \\ &A_k = \int_0^1 (\frac{3}{2} - s) e^{-s_k\tau(\sigma+1-s)} ds, \quad B_k = \int_0^1 (s - \frac{1}{2}) e^{-s_k\tau(\sigma+1-s)} ds. \end{aligned} \tag{12}$$

Here the coefficients s_k are the positive points, w_k are the weights, and the detailed derivations are given in [19]. The initial condition is spread to surrounding points using the discrete Dirac-delta function (10) as well.

4. Results and discussion

In this section, the effects of involved parameters (α, d_r, d_θ) on the marginal distribution function $P(1, \theta)$ and the MSD are investigated, and the memory effects with different values of fractional order α are discussed in detail. The MSD is computed as follows

$$\langle \theta^2(t) \rangle = \frac{\int_{-\pi}^{\pi} \theta^2 P(1, \theta, t) d\theta}{\int_{-\pi}^{\pi} P(1, \theta, t) d\theta}. \tag{13}$$

The mesh numbers are set as $N_r = 100$, $N_\theta = 600$, and the time step size is $\tau = 10^{-3}$. The tiny outward extension is set as $\epsilon = h_r/2$. To solve the resulting sparse system efficiently, we use the GMRES iterative method with a tolerance of 10^{-10} at each time step.

From Fig. $2(a)(d)$, as the fractional order α is decreased, the peak value rises while the distribution of both sides declines, and the longer time is required to achieve the uniform distribution which shows the stronger memory effects. Moreover, the MSD presents sublinear growth in time, and the growth rate gradually decreases. The effects of the radial and tangential mobilities on the $P(\theta)$ and MSD are displayed in Fig. 2$(b)(e)$ and Fig. 2$(c)(f)$, respectively. One can observe that the higher radial mobility leads to the larger $P(\theta)$ while the smaller MSD. The effects of tangential mobility exhibits opposite changes for the $P(\theta)$ and MSD.

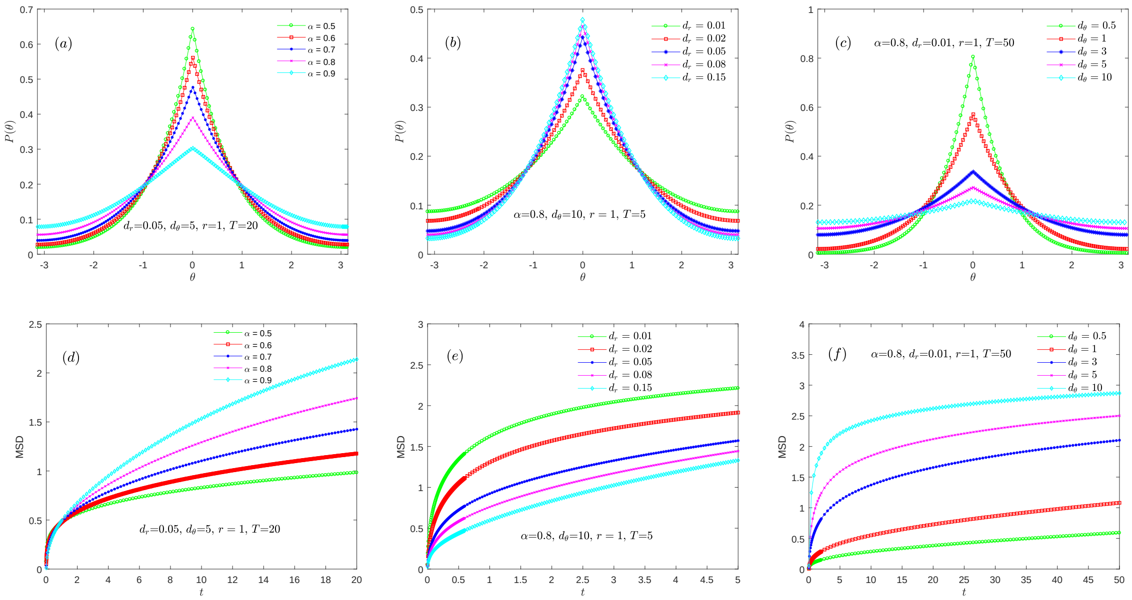

Fig. 2: Effects of the parameters (α, d_r, d_θ) on the marginal distribution $P(\theta)$ and MSD.

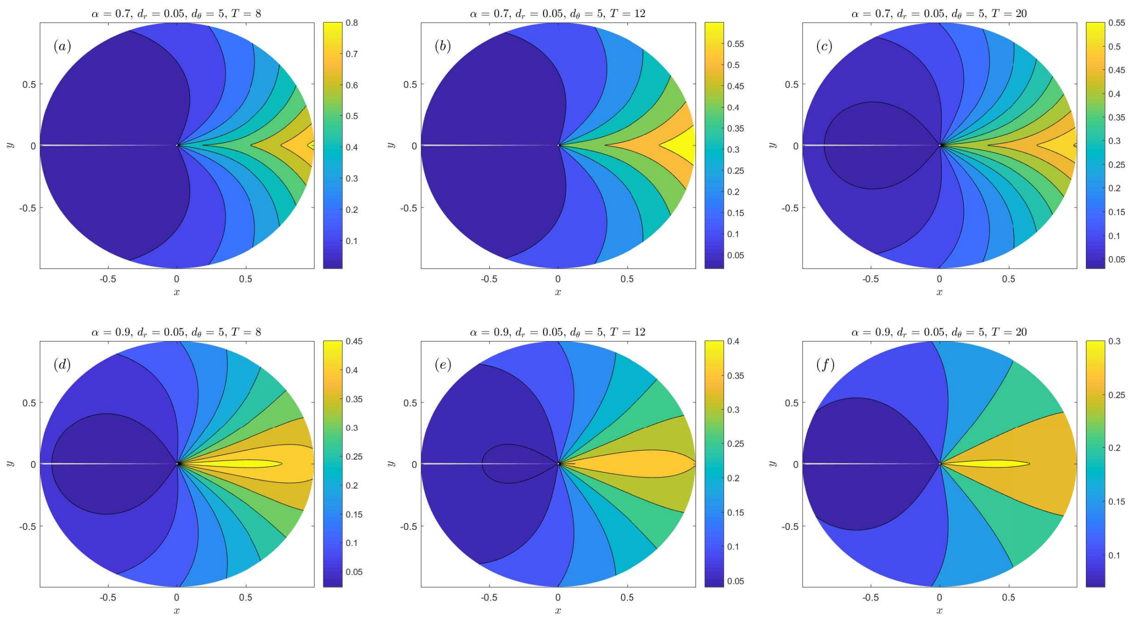

Fig. 3: Time evolution of the contour maps of P for different values of fractional order α.

In Figs. 3-5, we present the time evolution of P for different values of the fractional order α and the different ratios of the tangential mobility to the radial mobility. The value $\alpha = 0.7$ is shown in Fig. 3(a)-(c) and $\alpha = 0.9$ in Fig. 3(d)-(f). The results show that with the increase of α the particle diffusion is faster. The ratios of the tangential mobility to the radial mobility at $d_\theta/d_r = 10^2$ and $d_\theta/d_r = 10^3$ are presented in Fig. 4 and Fig. 5. We can see that with the increase of the tangential mobility the distribution function P achieves uniform distribution on the circle in a shorter time and the particles are more quickly to be spread to the interior of the circle.

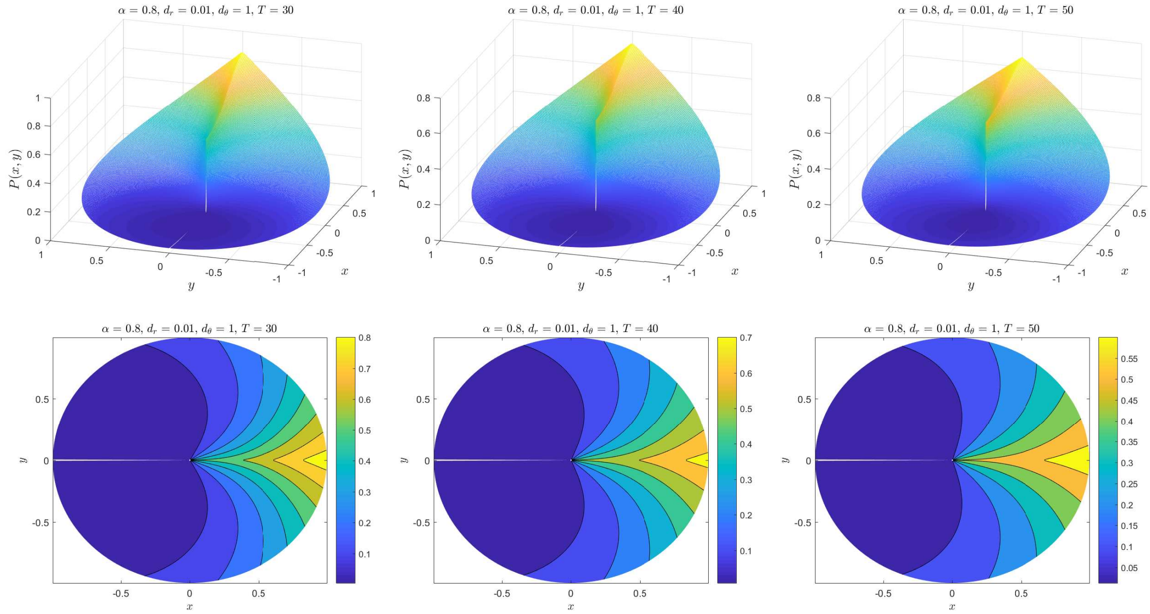

Fig. 4: Time evolution of P and the associated contour maps with the ratio $d_\theta/d_r = 10^2$.

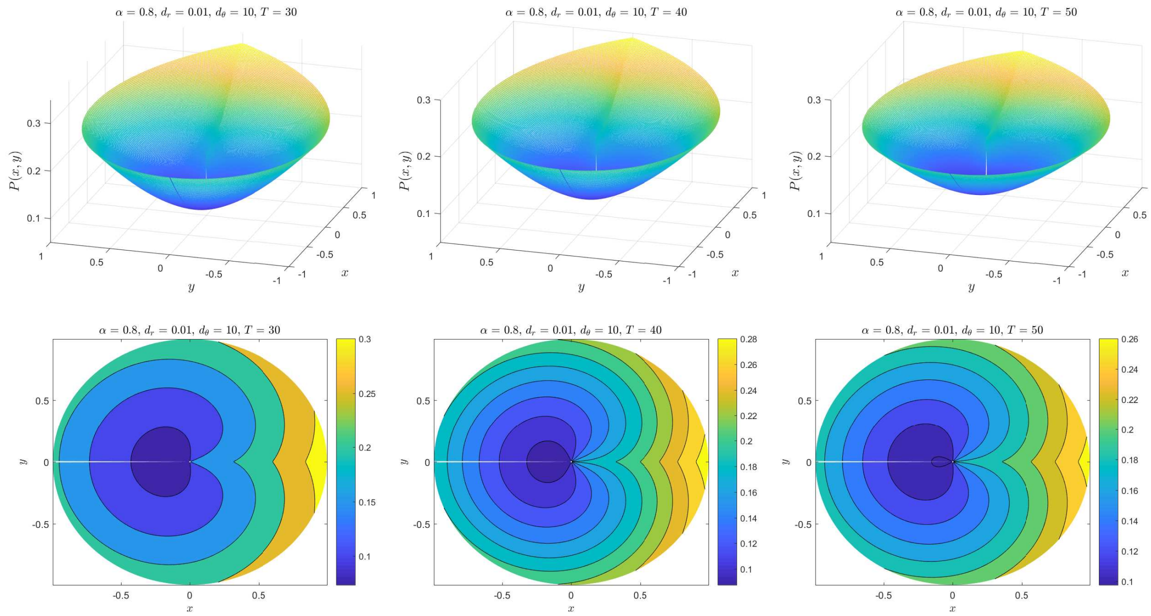

Fig. 5: Time evolution of P and the associated contour maps with the ratio $d_\theta/d_r = 10^3$.

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